

Argonne Leadership Computing Facility

Accelerating Discovery and Innovation

Katherine M Riley

Director of Science, Argonne Leadership Computing Facility

www.anl.gov

Supercomputing Resources

Our supercomputers are 10 to 100 times more powerful than systems typically used for scientific research.



Computing Resource for 2019



Theta Cray XC40 4,392 nodes 281,088 cores 892 TiB RAM Peak flop rate: 11.69 PF

Iota Intel/Cray XC40 44 nodes 2,816 cores 8.9 TiB RAM Peak flop rate: 117 TF Firestone IBM Power8 2 nodes + K80 GPU 20 cores 128 GB RAM Hybrid CPU/GPU Cooley Cray/NVIDIA 126 nodes 1512 Intel Haswell CPU cores 126 NVIDIA Tesla K80 GPUs 48 TB RAM / 3 TB GPU

Storage Capability Disk

 Theta: ~18 PB of GPFS/Lustre file system capacity; 9PB is GPFS and 9.2PB is Lustre.

Tape

 The ALCF has three 10,000-slot libraries using LTO 6 tape technology. The LTO tape drives have built-in hardware compression for an effective capacity of 36-60 PB.



Theta

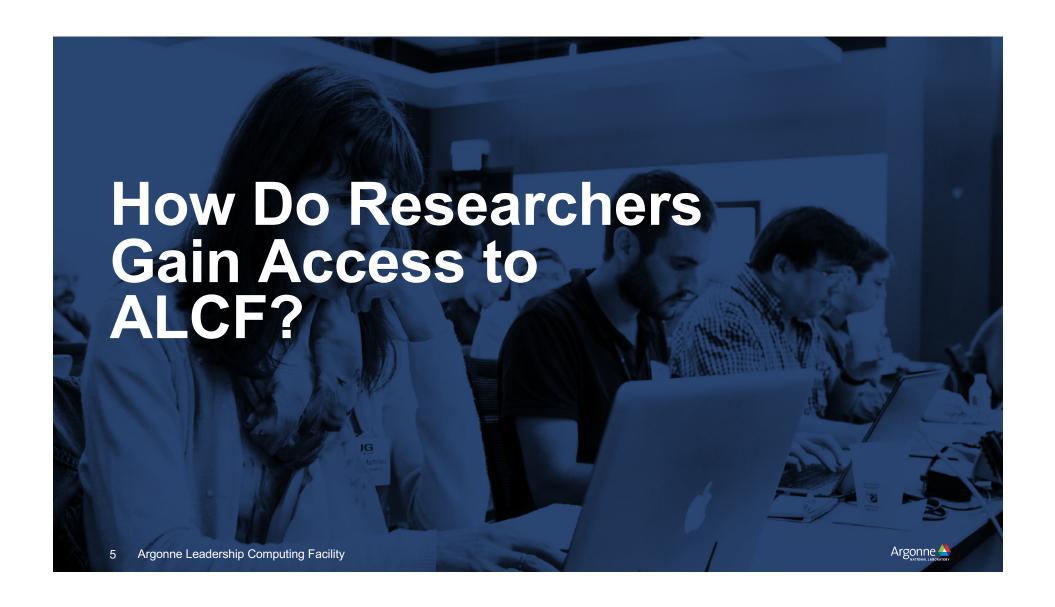
Features Intel
processors and
interconnect technology,
a new memory
architecture, and a
Lustre-based parallel
filesystem – all
integrated by Cray's
HPC software stack



Aurora : Nations First ≥1 Exaflop Supercomputer

Delivery in 2021 Intel Xeon scalable processors – Xe arch based GP-GPU Supporting the future of science Simulation Data Pre-planning < Design review IPR review Rebaseline Approved NRE contract award Build contract modification ALCF-3 Facility and Site Prep, Commissioning ALCF-3 ESP: Application Readiness NRE: HW and SW engineering and productization Build/Delivery/Acceptance CY 2018 CY 2022 CY 2017 CY 2019 CY 2020 CY 2021



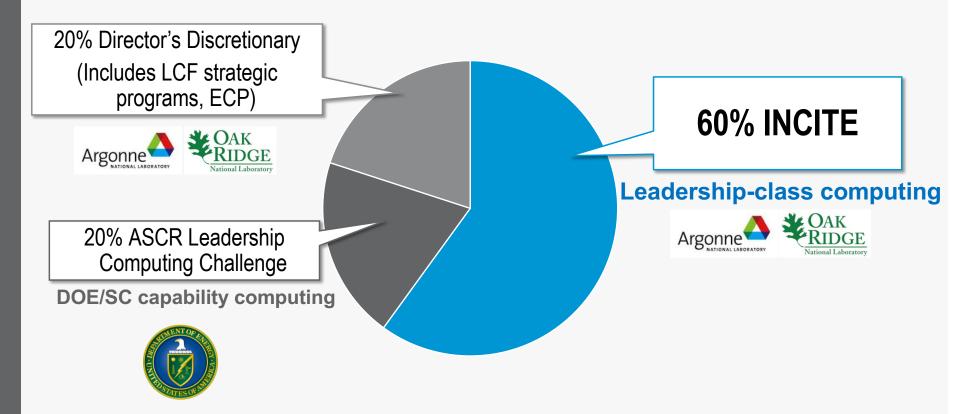


We offer different pipelines based on your computational readiness. Apply to the allocation program that fits your needs.

- Getting Started (DD)
- Major Awards (INCITE, ALCC)
- Targeted Projects (ADSP, ESP)



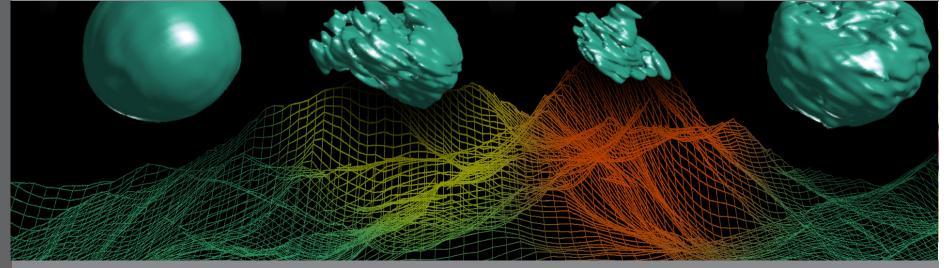
Primary Allocation Programs for Access to the LCFs Current distribution of allocable hours



Getting Started (DD)

Our Director's Discretionary (DD) allocation program provides researchers with small awards of computing time to "get started" on our computing resources while pursuing real scientific goals.

The DD allocation program allows users to prep their code so that it can take advantage of our massively parallel systems.



DD Director's Discretionary

Purpose: A "first step" for projects working toward a major allocation

Eligibility: Available to all researchers in academia, industry, and other

research institutions

Review Process: Projects must demonstrate a need for high-performance

computing resources; reviewed by ALCF

Award Size: Low 10 thousand of node-hours

Award Duration: 3-6 months, renewable

Total percent of ALCF resources allocated: 20%

Award Cycle

Ongoing (available year round)



ADSP

ALCF Data Science Program

Targeted at big data science problems, ADSP aims to explore and improve a variety of computational methods that will help enable data-driven discoveries across all scientific disciplines.

Eligibility: Available to researchers in academia, industry, and other research institutions

Review process: Applications undergo a review process to evaluate potential impact, data scale readiness, diversity of science domains and algorithms, and other criteria

Award size: ~Low hundred of thousand of node-hours

Award duration: 2 years

Award Cycle

October 1 to September 30



ESP Early Science Program

As part of the process of bringing a new supercomputer into production, the ALCF hosts the Early Science Program (ESP) to ensure its next-generation systems are ready to hit the ground running.

The intent of the ESP is to use the critical pre-production time period to prepare key applications for the architecture and scale of a new supercomputer, and to solidify libraries and infrastructure to pave the way for other production applications to run on the system.

In addition to fostering application readiness, the ESP allows researchers to pursue innovative computational science projects not possible on today's leadership-class supercomputers.

Award Cycle

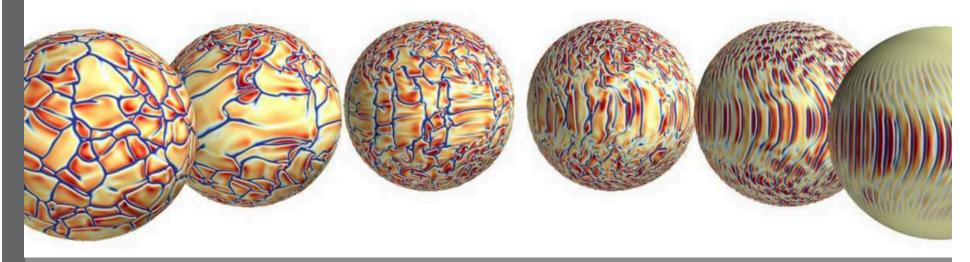
Determined by production timeline



Major Awards (INCITE, ALCC)

Our major allocations provides users with computationally intensive, large-scale research projects time on our machines.

The programs conduct a two-part review of all proposals: a peer review by a panel of experts and a computational readiness review.



INCITE

Innovative & Novel Computational Impact on Theory and Experiment

The DOE's INCITE program provides allocations to computationally intensive, large-scale research projects that aim to address "grand challenges" in science and engineering.

Eligibility: Available to researchers in academia, industry, and other research institutions

Review process: INCITE program conducts a two-part review of all proposals including a peer review by an international panel of experts, and a computational-readiness review

Award size: ~1.5-2.5M node-hours

Award duration: 1-3 years, renewable

Total percent of ALCF resources allocated: 60%

Award Cycle

January 1 to December 31



What is INCITE?



Innovative and Novel Computational Impact on Theory and Experiment

INCITE promotes transformational advances in science and technology through large allocations of computer time, supporting resources, and data storage at the Argonne and Oak Ridge Leadership Computing Facilities (LCFs) for computationally intensive, large-scale research

projects.

Argonne

♣OAK RIDGE

INCITE criteria

Access on a competitive, merit-reviewed basis*

Merit criterion

Research campaign with the potential for significant domain and/or community impact

Computational leadership criterion

Computationally demanding runs that cannot be done anywhere else: capability, architectural needs

Eligibility criterion

- Grant allocations regardless of funding source*
- Non-US-based researchers are welcome to apply

*DOE High-End Computing Revitalization Act of 2004: Public Law 108-423



Twofold review process

		New proposal assessment	Renewal assessment
2	Peer review: INCITE panels	 Scientific and/or technical merit Appropriateness of proposal method, milestones given Team qualifications Reasonableness of requested resources 	 Change in scope Met milestones On track to meet future milestones Scientific and/or technical merit
	Computational readiness review: LCF centers	Technical readinessAppropriateness for requested resources	 Met technical/ computational milestones On track to meet future milestones
	Award Decisions	INCITE Awards Committee comprise manager, LCF directors of science, s	

Recent Trends in INCITE

Data, Learning and Nontraditional Uses of the Architecture

In addition to traditional computationally intensive simulation campaigns, INCITE encourages Data and/or Learning projects with unique data requirements (e.g. large scale data analytics) or workflow needs that can only be enabled by the LCFs.

- A "Learning" panel evaluated proposals that had significant machine / deep learning component to their campaign
- These proposals were also assessed by their scientific discipline peers as well



2019 award statistics, by system

	Titan	Summit	Mira	Theta
Number of projects*	20	30	21	16
Average Project	1.95 M	457 K	10.5 M	1.11 M
Median Project	1.41 M	357 K	8.00 M	1.00 M
Total Awards (node- hrs in CY2016)	39.0 M	13.7 M	220 B	17.8 M

^{*} Total of 62 INCITE projects (many of the projects received time on a combination of Mira, Theta, Titan, and Summit)



^{**} All reported in node-hours nature to each resource.

New proposals,* new Pl's

*excluding renewal submittals

38% of the PI's had never before led an INCITE proposal

- -104 new proposals, 41 led by new Pl's
- 20% of non-renewal projects awarded time led by new Pl's
 - -41 new projects awarded, 8 led by new Pl's

INCITE actively engages with new research teams through outreach such as workshops, email distributions, and individual networking.



ALCC ASCR Leadership Computing Challenge

The DOE's ALCC program allocates resources to projects directly related to the DOE's energy mission, as well as national emergencies, and for broadening the community of researchers capable of using leadership computing resources.

Eligibility: Available to researchers in academia, industry, and other research institutions

Review process: DOE peer reviews all proposals for scientific/technical merit; appropriateness of approach; and adequacy of personnel and proposed resources

Award size: ~1M node-hours

Award duration: 1 year

Total percent of ALCF resources allocated: 20%

Award Cycle July 1 to June 30



LCF Allocation Programs	IN	CITE 60	%	Al	LCC 20%		ector's 20% etionary
Mission	High-risk, high-payoff science that requires LCF-scale resources*		High-risk, high-payoff science aligned with DOE mission		50% Strategic LCF goals 50% ECP		
Call	1x/year – (Closes June) 2019 Call Open		1x/year – Closes February		Rolling		
Duration	1-3 years, yearly renewal		1 year		3m,6m,1 year		
Typical Size	10-15 projects	1-3M node-hour	S	10-15 projects	0.5-2M node- hours	~100 of projects	<0.5M node- hours
Total Hours	~17.8M Theta		~6M node-hours Theta		~6M node-hours Theta		
Review Process	Scientific Peer-Review	Computational Readiness		Scientific Peer-Review	Computational Readiness	Strategic impact and feasibility	
Managed By	INCITE management committee (ALCF & OLCF)		DOE Office of Science		LCF management		
Readiness	High		Medium to High		Low to High		
Availability	Open to all scientific researchers and organizations Capability > 20% of resource						

Targeted Projects (ADSP, ESP)

Our ADSP program is intended for projects hoping to gain insight into very large datasets produced by experimental, simulation, or observational methods.

Our ESP program is intended to help ready our next-generation supercomputers for production.

